

(purple atoms). At later times we observe the nucleation of $\langle 100 \rangle$ slip, predominantly at the intersection of $1/2\langle 111 \rangle$ loops. We find that the plastic wave moves at the same speed of the shock front. For shocks in the $\langle 111 \rangle$ direction plastic deformation also begins with the nucleation of $1/2\langle 111 \rangle$ loops, but in this case the nucleation of the second $1/2\langle 111 \rangle$ loops inside the original ones lead to $\langle 100 \rangle$ slip (red atoms). In this case, the plastic wave does not catch up with the shock front: the plastic wave propagates slower than the shockwave and an elastic precursor develops. Finally, for loading in the $\langle 100 \rangle$ direction we observe multiple, almost simultaneous, nucleation of $1/2\langle 111 \rangle$ loops and the frequent intersection thereof; this entanglement severely limits their mobility and even leads to local amorphization.

In summary, we used MD simulations to characterize the details of the plastic response of NiAl single crystals under compressive uniaxial loading. While in all cases plastic deformation starts with the nucleation of $1/2\langle 111 \rangle$ loops, the subsequent phenomena exhibits marked anisotropy. Shocks in $\langle 110 \rangle$ have a single wave structure with the plastic wave traveling at the shock speed; on the other hand for $\langle 111 \rangle$ and $\langle 100 \rangle$ loading we find a two-wave structure with the plastic wave following an elastic precursor.

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